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Dynamic 1H, 13C, 31P NMR spectroscopy of the crown containing N-(thio)phosphoryl(thio)urea

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Abstract

The variable temperature and concentration 1H, 13C, 31P NMR spectroscopy of the N,N′-bis[diisopropoxy(thio)phosphorylamido-(thio)carbonyl]-1,10-diaza-18- crown-6 containing the reaction pentade C(X)NHP(Y) and stereononrigid macrocycle in solutions (CD2CL2, CD3CN, (CD3)2CO as solvent) was studied. The complex chemical exchange is described in terms of tautomeric processes, hindered rotation around C-N bond and macrocycle ring inversion. NMR spectral parameters (chemical shifts and spin-spin coupling constants) of the observed exchange partners as well as thermodynamic parameters of the equilibrium and transition between tautomeric and conformational forms are given.